High-Temperature Expansion of the Free Energy in the Two-Dimensional XY Model

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We extend the high-temperature series of the free energy for the XY model in two dimensions to order β^{48} from the previous order of β^{22} by applying an improved algorithm of the finite lattice method. The long series obtained allows us to conclude that the behavior of the free energy is consistent to high accuracy with what is expected when the phase transition of the model is of the Kosterlitz-Thouless type.

§1. Introduction

We investigate the XY model in two dimensions. It is believed to exhibit a phase transition of the Kosterlitz-Thouless (K-T) type,[1] driven by the condensation of vortices. Through use of renormalization group arguments, it was predicted that the correlation length possesses an essential singularity at the transition temperature T_c of the form

$$\xi \sim \exp\left[\frac{b}{t^{1/2}}\right], \tag{1·1}$$

where $t = T/T_c - 1$ is the reduced temperature and b is a non-universal constant. The free energy and its temperature derivatives (i.e., the internal energy and the specific heat) have also been predicted to behave as

$$f \sim \exp\left[-\frac{2b}{t^{1/2}}\right] + [\text{ a regular term}]. \tag{1·2}$$

The first term on the right-hand side of Eq. (1·2) has an essential singularity at $t = 0$. This term itself and its derivatives are zero at the critical temperature. The second term is regular at the critical temperature.

The behavior expressed in (1·1) for the correlation length has been well established both by numerical simulations and the high-temperature expansion. The standard Monte Carlo simulation[2],[3] gives $b = 2.15(10)$ with $\beta_c = 1.130(15)$ and $b = 1.70(20)$ with $\beta_c = 1.118(5)$ for the square lattice. (Here β_c is the inverse critical temperature, which is defined below.) The more precise values $b = 1.800(2)$ with $\beta_c = 1.1208(2)$ and $b = 1.776(4)$ with $\beta_c = 1.1199(1)$ were obtained using the finite-size scaling technique[4] and the renormalization group finite-size scaling method,[5] respectively. In the latter approach, the renormalization group flow of the observable was matched with that of the exactly solvable BCSOS model. The latter value of β_c was recently confirmed by large scale Monte Carlo simulations on a 2048×2048 lattice using the finite-size scaling method.[6] A high-temperature expansion for the correlation length[7],[8] gives the slightly smaller value $b = 1.67(4)$ with $\beta_c = 1.118(3)$.

In contrast to the situation for (1·1), the behavior expressed by (1·2) for the free energy or its temperature derivatives has not yet been confirmed in numerical simulations or in high-temperature expansions. The reason for this is the following. The free energy and its derivatives are dominated by the regular term near the critical temperature, and the signal of the singularity in the first term is relatively weak. For this reason, a much more precise simulation is needed to confirm the behavior given in (1·2) for these quantities than in the case of the correlation length. For the high-temperature expansion also, the presence of the regular term in (1·2) makes it difficult to use standard analyzing methods of the series (such as the Padé approximation and the inhomogeneous differential approximation) to pick out the singular term. However, we believe that the contribution of the singular term to the coefficients in the high-temperature series will dominate at sufficiently high orders. If this is indeed the case, we could directly compare the high-temperature series of the free energy with an expansion series of a form like that of the first term on the right-hand side of Eq. (1·2) if we calculate a sufficiently long series for the free energy. In this paper, we extend the previously derived high-temperature series for the free energy[8] to a series that is more than two times longer. This makes it possible to reveal the singular behavior of Eq. (1·2). From an analysis of the obtained series we obtain the value of $\beta_c = 1.1176(33)$ for the inverse critical temperature and $b = 1.54(4)$ for the non-universal constant in Eq.(1·2).

A commonly used method for series expansions is the graphical method.[9] However, in this method, one must list all the graphs that contribute to the desired order of the series. An alternative, powerful method to generate the expansion series is the finite lattice method.[10],[11],[12] It does not require that we list the graphs and it reduces the problem to that of calculating the partition functions for the relevant finite-size lattices. This is a rather straightforward procedure if we use the transfer matrix formulation. In many cases, the finite lattice method generates longer series than the graphical method.[13],[14],[15],[16],[17],[18],[19],[20] Unfortunately, the original finite lattice method can generate a high-temperature series that is at most as long as that which can be obtained with the graphical method in the case of the XY model in two dimensions.

Here we apply an improved algorithm of the finite lattice method developed by the author and Tabata[21],[22] to generate a long series for the the XY model in two dimensions. This improved algorithm is powerful in the case of models in which the spin variable at each site takes more than two values, including the case that it takes an infinite number of values. This algorithm was applied to generate a low-temperature series for the absolute value solid-on-solid (ASOS) model and high- and low-temperature series for the q-state Potts model in two dimensions. In both cases, it generates much longer series than the original finite lattice method. The XY model in two dimensions can be mapped to a kind of solid-on-solid model, and the improved algorithm of the finite lattice method enables us to obtain a series that is two times longer than the series previously derived for the free energy. We confirm from analysis of the obtained long series that the free energy of the two-dimensional XY model behaves like Eq. (1·2), with values of the critical temperature and the non-universal constant b that are close to the values obtained in studies of

the correlation length.

§2.   Algorithm

We consider the XY model defined on the square lattice. The Hamiltonian of this system is

$$H = -\sum_{\langle i,j \rangle} J \vec{s}_i \vec{s}_j \;, \tag{2·1}$$

where $\vec{s}_i$ is a two-dimensional unit vector located at the lattice site i, and the summation is taken over all the pairs $\langle i, j \rangle$ of nearest neighbor sites. The partition function at temperature T is

$$Z = \int \prod_i d\theta_i \exp\left(-\frac{H}{kT}\right) \;, \tag{2·2}$$

where θ_i is the angle variable of the spin $\vec{s}_i = (\cos\theta_i, \sin\theta_i)$. This model can be mapped exactly to a solid-on-solid model whose partition function is

$$Z = \sum_{\{h \,|\, -\infty \leq h_i \leq +\infty\}} \prod_{\langle i,j \rangle} I_{|h_i - h_j|}(\beta) \;,$$

where $\beta = \frac{J}{kT}$, the quantities I_n are modified Bessel functions, the product is taken with respect to all the pairs of neighboring plaquettes, and the variable h_i at each plaquette i takes an integer value between $-\infty$ and $+\infty$.

The improved algorithm of the finite lattice method to generate the high-temperature expansion series for the free energy of this model employed here is the following. We first calculate the partition function for each of the $l_x \times l_y$ finite-size rectangular lattices with a restricted range of the values of the plaquette variables $\{h\}$:

$$Z(l_x, l_y; h_+, h_-) = \sum_{\{h \,|\, h_- \leq h_i \leq h_+\}} \prod_{\langle i,j \rangle} I_{|h_i - h_j|}(\beta) \;. \tag{2·3}$$

Here, each plaquette variable h_i is restricted as $h_- \leq h_i \leq h_+$ (where $h_- \leq 0$ and $h_+ \geq 0$). We define the size of the finite lattice so that an $l_x \times l_y$ lattice involves $l_x \times l_y$ plaquettes, including the bonds and sites on their boundary. For instance, the 1×1 lattice consists of a single plaquette, including 4 bonds and 4 sites. We take into account finite-size lattices with $l_x = 0$ and/or $l_y = 0$. An $l_x \times 0$ lattice consists of l_x bonds and $l_x + 1$ sites with no plaquette. The 0×0 lattice consists only of one site with no bond or plaquette. We take the boundary condition such that all the plaquette variables outside the $l_x \times l_y$ lattice are fixed to zero.

We then define W of the $l_x \times l_y$ lattice and of the restricted range of the plaquette variables recursively as

$$\begin{aligned}
W(l_x, l_y; h_+, h_-) = &-\log Z(l_x, l_y; h_+, h_-) \\
&- \sum_{\substack{0 \leq l'_x \leq l_x,\ 0 \leq l'_y \leq l_y,\ 0 \leq h'_+ \leq h_+,\ h_- \leq h'_- \leq 0, \\ l'_x \neq l_x,\ l'_y \neq l_y\ h'_+ \neq h_+,\ h'_- \neq h_-}} (l_x - l'_x + 1)(l_y - l'_y + 1) W(l'_x, l'_y; h'_+, h'_-).
\end{aligned}$$
$$\tag{2·4}$$

The initial form of $W(l_x, l_y; h_+, h_-)$ is as follows:

$$Z(0, 0; h_+, h_-) = 1 \quad \text{and} \quad W(0, 0; h_+, h_-) = 0. \tag{2.5}$$

$$Z(l_x, 0; h_+, h_-) = Z(l_x, 0; 0, 0) = I_0(\beta)^{l_x} \quad \text{for} \quad l_x \geq 1 \quad \text{and}$$

$$W(l_x, 0; h_+, h_-) = \begin{cases} -\log I_0(\beta) & \text{for } l_x = 1 \text{ and } h_+ = h_- = 0, \\ 0 & \text{for } l_x \geq 2 \text{ or } h_+ \geq 1 \text{ or } h_- \leq -1. \end{cases} \tag{2.6}$$

$$Z(1, 1; h_+, h_-) = \sum_{h=h_-}^{h_+} I_{|h|}(\beta)^4 \quad \text{and}$$

$$W(1, 1; 0, 0) = -\log Z(1, 1; 0, 0) - 2W(1, 0; 0, 0) - 2W(0, 1; 0, 0) - 4W(0, 0; 0, 0)$$
$$= -\log I_0(\beta)^4 + 4\log I_0(\beta) = 0.$$

$$W(1, 1; 1, 0) = -\log Z(1, 1; 1, 0) - W(1, 1; 0, 0) - 2W(1, 0; 1, 0) - 2W(1, 0; 0, 0)$$
$$\qquad -2W(0, 1; 1, 0) - 2W(0, 1; 0, 0) - 4W(0, 0; 1, 0) - 4W(0, 0; 0, 0)$$
$$= -\log\{I_0(\beta)^4 + I_1(\beta)^4\} + 4\log I_0(\beta)$$
$$= -\log\left[1 + \left\{\frac{I_1(\beta)}{I_0(\beta)}\right\}^4\right] = O(\beta^4). \tag{2.7}$$
$$\cdots$$

The free energy density f_s per site in the infinite-volume limit is given by

$$f_s = \sum_{l_x, l_y, h_+, h_-} W(l_x, l_y; h_+, h_-). \tag{2.8}$$

In the standard (graphical) cluster expansion of the free energy for this model, a cluster is composed of polymers, and each of the polymers consists of connected plaquettes. An example of a polymer can be seen in Fig. 1. A value h_i $(\neq 0)$ is assigned to each site i of the polymer. We can assign to each cluster two numbers, $h_{\max}$ (≥ 0) and $h_{\min}$ (≤ 0), which are the maximum and the minimum, respectively, of the quantities h_i in all the sites of the polymers of which the cluster consists. Then, we can prove[11] that the Taylor expansion of $W(l_x, l_y; h_+, h_-)$ with respect to
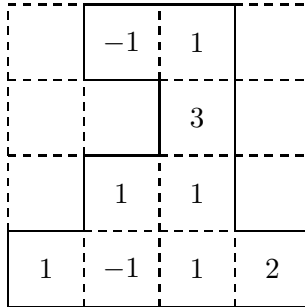

Fig. 1.   An example of a polymer in the standard cluster expansion.

β includes the contributions from all the clusters of polymers in the standard cluster expansion for which $h_{\max} = h_+$ and $h_{\min} = h_-$ and that can be embedded into the $l_x \times l_y$ lattice but cannot be embedded into any of its rectangular sub-lattices. The series expansion of $W(l_x, l_y; h_+, h_-)$ begins at order $\beta^{n(l_x, l_y, h_+, h_-)}$, with

$$n(l_x, l_y, h_+, h_-) = \begin{cases} 2(l_x + l_y) + 4(h_+ + |h_-|) - 6 & \text{for } h_+ > 0 \text{ and } h_- < 0, \\ 2(l_x + l_y) + 4(h_+ + |h_-|) - 4 & \text{for } h_+ = 0 \text{ or } h_- = 0. \end{cases}$$

(2·9)

An example of a cluster consisting of a single polymer that contributes to the lowest-order term of $W(l_x, l_y; h_+, h_-)$ is given in Fig. 2. Hence, to obtain the expansion series to order β^N, we have only to take into account all combinations of the rectangular lattice size (l_x, l_y) and the range of the plaquette variables (h_+, h_-) that satisfy the relation $n(l_x, l_y, h_+, h_-) \le N$ in the summation of Eq. (2·8) and to evaluate each of the $W(l_x, l_y, h_+, h_-)$ to order β^N.
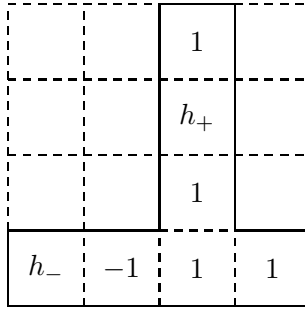

Fig. 2.   An example of a cluster consisting of a single polymer that contributes to the lowest-order term of $W(l_x, l_y; h_+, h_-)$ with $l_x = l_y = 4$, $h_- < 0$ and $h_+ > 0$.

Most of the CPU time required with this algorithm is used for the calculation of the relevant partition functions $Z(l_x, l_y; h_+, h_-)$ to order β^N. These partition functions are calculated with the transfer matrix method using a procedure in which a finite-size lattice is built one plaquette at a time.[23), 24)] The necessary CPU time and memory are proportional to $N l_x l_y (h_+ + |h_-| + 1)^{\min(l_x, l_y)}$ and $N (h_+ + |h_-| + 1)^{\min(l_x, l_y)}$, respectively.

If we had applied the original finite lattice method straightforwardly, without introducing h_+ and h_-, we would have had to calculate the partition function while taking into account all the configurations with each of the plaquette variables ranging from $-N/4$ to $N/4$ for any necessary size of the lattice. However, because we have introduced h_+ and h_-, we only need to take into account the configurations with each of the plaquette variable ranging between h_- and h_+, with $|h_-| + h_+ \le (N - 2(l_x + l_y))/4$. This substantially reduces the number of the configurations that have to be taken into account, especially for larger lattices. In fact, if we had used the original method, we would have been able to generate a high-temperature series only to order β^{24}, instead of β^{48}.

§3. Series

We have calculated the high-temperature expansion series for the free energy of the XY model on the square lattice to order β^{48}. The obtained coefficients for the free energy f_b per bond are listed in Table I, where the quantities a_n are defined through the relation

$$f_b = \frac{f_s}{2} = \sum_{n=1}^{N} a_n \left(\frac{\beta}{2}\right)^n . \tag{3·1}$$

We have confirmed that each $W(l_x, l_y; h_+, h_-)$ in Eq. (2·8) starts from the correct order in β, as given by Eq. (2·9). The first eleven terms of the series (to order β^{22}) coincide with those obtained by Campostrini et al.,[8] and we have generated thirteen new terms.

To obtain the long numerators and denominators appearing in Table I precisely, we have used the following technique. The Taylor series of the Bessel function $I_n(\beta)$

Table I. High-temperature series coefficients for the free energy per bond of the XY model on the square lattice.

n	a_n
2	-1
4	$-3 \,/\, 4$
6	$-1 \,/\, 9$
8	$31 \,/\, 192$
10	$731 \,/\, 600$
12	$29239 \,/\, 8640$
14	$265427 \,/\, 35280$
16	$75180487 \,/\, 5160960$
18	$6506950039 \,/\, 235146240$
20	$1102473407093 \,/\, 26127360000$
22	$6986191770643 \,/\, 158070528000$
24	$-1657033646428733 \,/\, 49662885888000$
26	$-132067307951625029 \,/\, 349709488128000$
28	$-123922162516396049161 \,/\, 73815602724864000$
30	$-3988676736069063737749 \,/\, 684416646144000000$
32	$-171797935005592667747929271 \,/\, 9718351353033523200000$
34	$-444707272848202938952537383 \,/\, 8776886065708400640000$
36	$-14198693740026507460964360083 43 \,/\, 1003662735984537108480000 0$
38	$-37739166891866120573923814513909 \,/\, 100645068802893860044800000$
40	$-7997230785639084542407519918030 0349 \,/\, 8475374214980535582720000 0000$
42	$-3529608673175063035175810323068581713 \,/\, 15094315500949888467609600 00000$
44	$-5592178761750017673515079712502627 4875543 \,/\, 994959775668267990304948224 0000000$
46	$-147044539813816049655151587938971 4706601279$ $/\, 119621300301934947016208547840000000$
48	$-703381237258093332090416384961669820 4389178239$ $/\, 287590409630251949139489907015680000000$

can be written

$$I_n(\beta) = \sum_i \frac{b_{n,i}}{i!} \left(\frac{\beta}{2}\right)^i , \tag{3.2}$$

where the coefficients $b_{n,i}$ are all integers. The product of two Bessel functions can also be written as

$$I_{n_1}(\beta)I_{n_2}(\beta) = \sum_i \frac{c_i}{i!} \left(\frac{\beta}{2}\right)^i , \tag{3.3}$$

with

$$c_i = \sum_{i'=0}^i \frac{i!}{i'!(i-i')!} b_{n_1,i'} b_{n_2,i-i'} . \tag{3.4}$$

We note that the combinatorial factor $\frac{i!}{i'!(i-i')!}$ is an integer and that c_i is also an integer. Thus, if we treat coefficients like $b_{n,i}$ and c_i in Eqs. (3.2) and (3.3) instead of the coefficients of the terms in the Taylor expansion, then we need only treat integer values throughout the calculation. For the products and summations of the long integers that arise in these calculations, we used the Chinese theorem of modulus.[14]

The calculations were carried out on a workstation at the Information Processing Center at OPCT and on an Altix3700 BX2 at YITP of Kyoto University.

§4.   Series analysis

If the phase transition of the model is of K-T type, the free energy is expected to behave as

$$f(\beta) = A\beta^2 \exp\left[-\frac{2b}{(1-\beta/\beta_c)^{1/2}}\right] + B(\beta), \tag{4.1}$$

where β_c is the inverse critical temperature and $b\ (>0)$ is the non-universal constant that appears in Eqs. (1.1) and (1.2).

First, it is to be noted that the coefficients of the free energy in Table I exhibit repeated changes of sign. This is one indication that the phase transition in this model is of the Kosterlitz-Thouless type. This property of the signs of the coefficients in the expansion series of the free energy for a model that undergoes a K-T type phase transition was first pointed out by Hasenbusch et al.[25] The coefficients in the Taylor expansion of the first term on the right-hand side of Eq. (4.1) with respect to β exhibits repeated changes of sign in general, with the order of the sign change depending on the values of c and β_c, while the coefficients of the terms in the Taylor expansion for a quantity with a power law singularity do not exhibit changes of sign. In fact, changes in sign of the coefficients is observed in the low-temperature series for the surface free energy of the Ising model (i.e., the strong coupling series for the string tension of the Z_2 lattice gauge theory) in three dimensions[15] and also in the low-temperature series of the free energy for the ASOS model in two dimensions,[25,21] both of which undergo a roughening phase transition of the K-T type.

It is expected that the coefficients of the terms in the series expansion of the free energy at sufficiently high orders will be dominated by the contribution from the

Taylor expansion of the first singular term in Eq. (4·1). With this in mind, rewriting the high-temperature series as

$$f = \sum_{n=1}^{N/2} \tilde{a}_n x^n \qquad \left(x = \left(\frac{\beta}{\beta_c} \right)^2 \right) , \tag{4·2}$$

we fit the K-T type function

$$f^{(\text{K-T})}(x) = A\,x \exp\left[-\frac{c_0 + c_1 x}{(1-x)^\sigma} \right] = \sum_n \tilde{a}_n^{(\text{K-T})} x^n \tag{4·3}$$

to the high-temperature series under the condition that

$$\frac{\sum_{n=n_0}^{N/2} (\tilde{a}_n^{(\text{K-T})} - \tilde{a}_n)^2}{\sum_{n=n_0}^{N/2} \tilde{a}_n^2} \tag{4·4}$$

be minimized. In the present case, we have $N/2 = 24$, and we have carried out the fitting for n_0 ranging from 7 to 13.

We have performed three types of fittings. We first fixed the exponent σ to $1/2$. In this case, the best fitting parameter values are $\beta_c = 1.1176(33)$, $c_0 = 2.86(25)$ and $c_1 = 1.50(18)$. The uncertainty on each value is due to the range of the values of n_0 adopted. This best fitting value of the inverse critical temperature is consistent with the most precise value $\beta_c = 1.1199(1)$, obtained from the large-scale Monte Carlo simulation,[6] and the value $\beta_c = 1.116(4)$ obtained from the high-temperature series for the correlation length and the magnetic susceptibility.[8],[7] Although the values of c_0 and c_1 have rather large uncertainties, the combination $c_0 + c_1$, which we find to be $4.36(11)$, has a smaller uncertainty. This is because the value of the quantity in Eq. (4·4) is stable on any line defined by $c_0 + c_1 = $ [constant] near the minimum
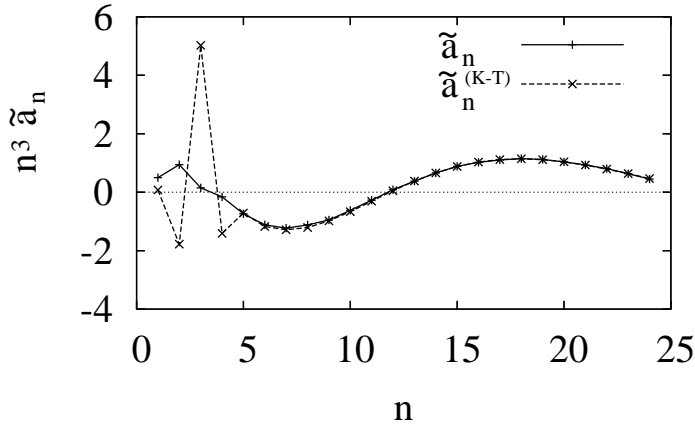

Fig. 3.   The coefficients $\tilde{a}_n$ and $\tilde{a}_n^{(\text{K-T})}$ multiplied by n^3.

point. In Fig. 3 we plot $\tilde{a}_n$ and $\tilde{a}_n^{(\text{K-T})}$ corresponding to the best fitting values of β_c, c_0 and c_1 for $n_0 = 13$. We find that the agreement between the two series is good not only in the range $13 \leq n \leq 24$ used in the fitting but also in the range $5 \leq n \leq 12$, which was not used in the fitting. This confirms the validity of our assumption that the series $\tilde{a}_n$ for sufficiently large n is dominated by the Taylor expansion of the first term in Eq. (4·1).

Next, we fixed the inverse critical temperature β_c to 1.1199. In this case, the fitting yields $\sigma = 0.513(19)$, and $c_0 + c_1 = 4.18(23)$. This best fitting value of σ is also consistent with the K-T value of $1/2$.

Finally, we set σ to $1/2$ and β_c to 1.1199. In this case, we obtained $c_0 + c_1 = 4.36(11)$. Here, the behavior of the coefficients $\tilde{a}_n$ and $\tilde{a}_n^{(\text{K-T})}$ with respect to n is almost the same as that plotted in Fig.3. The fitted values of the parameters c_0 and c_1 imply that the non-universal constant b in Eq. (1·2) is given by $(c_0 + c_1)/2\sqrt{2} = 1.54(4)$. We can see that the value of b obtained from the high-temperature series for the free energy is consistent with the value obtained from the Monte Carlo simulation of the correlation length to a precision of 15% and with the value obtained from the high-temperature series of the correlation length to a precision of 10%.

§5. Summary

We have calculated the high-temperature series for the free energy of the XY model on the square lattice to order β^{48} using an improved finite-lattice method. This method in general enables us to generate a longer expansion series for spin systems whose spin variable takes more than two values. The length of the series obtained here is two times longer than the series obtained previously with the graphical method. The results of the analysis for the obtained series give strong support to the validity of the prediction given in Eq.(1·2) for the behavior of the free energy of the XY model in two dimensions. The value of the critical point derived from the series for the free energy is consistent with the value obtained in studies of the correlation length employing the numerical simulations and series expansions. The value of the non-universal constant obtained from the series for the free energy is close to the value obtained from the correlation length. These results reconfirm that the phase transition of the model is of the Kosterlitz-Thouless type, which was first found in a study of the correlation length.

Acknowledgements

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